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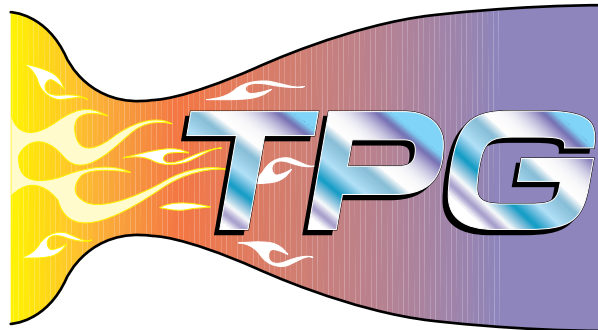
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Abstract

A set of compressible flow relations for a thermally perfect, calorically imperfect gas are derived for a value of c_p (specific heat at constant pressure) expressed as a polynomial function of temperature and developed into a computer program, referred to as the Thermally Perfect Gas (TPG) code. The code is available free from the NASA Langley Software Server at URL

<http://www.larc.nasa.gov/LSS>. The code produces tables of compressible flow properties similar to those found in NACA Report 1135. Unlike the NACA Report 1135 tables which are valid only in the calorically perfect temperature regime the TPG code results are also valid in the thermally perfect, calorically imperfect temperature regime, giving the TPG code a considerably larger range of temperature application. Accuracy of the TPG code in the calorically perfect and in the thermally perfect, calorically imperfect temperature regimes are verified by comparisons with the methods of NACA Report 1135. The advantages of the TPG code compared to the thermally perfect, calorically imperfect method of NACA Report 1135 are its applicability to any type of gas (monatomic, diatomic, triatomic, or polyatomic) or any specified mixture of gases, ease-of-use, and tabulated results.

Introduction

The traditional computation of the one-dimensional (1-D) compressible flow gas properties is performed with one-dimensional calorically perfect gas equations such as those of NACA Report 1135¹. If the gas of interest is air, then the tables of compressible flow values provided in NACA Report 1135 can be used. These tables were generated using the calorically perfect gas equations with a value of 1.40 for the ratio of specific heats, γ . The application of these equations and tables is limited to that range of temperature for which the calorically perfect gas assumption is valid. However, a significant number of aeronautical engineering calculations extend beyond the temperature limits of the calorically perfect gas assumption, and the application of the tables of NACA Report 1135 can result in significant errors. The temperature range limitation is greatly minimized by the assumption of a thermally perfect, calorically imperfect gas in the development of the compressible flow relations. (For the sake of terminology simplicity, throughout this paper the term "thermally perfect" will be used to denote a thermally perfect, calorically imperfect gas.) The purpose of this paper is to present a computer code which implements one-dimensional compressible flow relations derived for a thermally perfect gas.

A calorically perfect gas is by definition a gas for which the values of specific heat at constant pressure, c_p , and specific heat at constant volume, c_v , are constants. Therefore, in the derivation of the compressible flow relations for a calorically perfect gas, the value of c_p was

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assumed constant. The resulting calorically perfect gas equations are derived in many compressible flow textbooks and are summarized in NACA Report 1135. The accuracy of these equations is only as good as the assumption of a constant c_p (and therefore a constant γ). For any diatomic or polyatomic gas, the value of c_p actually varies with temperature and can only be approximated as a constant over some relatively small temperature range. At some point, as the temperature increases, the c_p value starts increasing appreciably due to the excitation of the vibrational energy of the molecules. This phenomena occurs around 450 to 500 K for air. Thus, above 500 K use of $\gamma = 1.40$ for air in the calorically perfect gas equations will yield noticeably incorrect results. The variation of c_p with temperature (and with only temperature) continues for air up to roughly 1500 K. In this temperature range, where the value of c_p is only a function of temperature, air is considered a thermally perfect gas. The derivation of the compressible flow relations for a thermally perfect gas therefore must account for a variable heat capacity. Above 1500 K for air, and at some relatively high temperature for all diatomic and polyatomic gases, dissociation of the molecules starts to occur. When dissociation commences, the value of c_p becomes a function of both temperature and pressure and the gas is no longer considered thermally perfect. The reason for specifically citing the calorically perfect and thermally perfect temperature limits for air is to illustrate the much larger temperature range of application available from a thermally perfect compressible flow analysis.

NACA Report 1135 presents one method for computing the one-dimensional compressible flow properties of a thermally perfect gas. In this approach the variation of heat capacity due to the contribution from the vibrational energy mode of the molecule is determined from quantum mechanical considerations through the assumption of a simple harmonic vibrator model of a diatomic molecule. With this assumption the vibrational contribution to the heat capacity of a diatomic gas takes the form of ²

$$\left(\frac{c_p}{R}\right)_{\text{vib}} = \left(\frac{\Theta}{T}\right)^2 \frac{e^{\frac{\Theta}{T}}}{\left(e^{\frac{\Theta}{T}} - 1\right)^2} \quad (1)$$

where R is the specific gas constant, $\Theta = hv/k$, h is

Planck's constant, ν is the characteristic frequency of molecular vibration, k is the Boltzmann constant, and T is the static temperature. The complete set of thermally perfect compressible flow relations based upon the c_p variation given in equation (1) are listed in NACA Report 1135 in the section entitled "Imperfect-Gas Effects". Tables of these thermally perfect gas properties are not provided because each value of total temperature, T_t , would yield a unique table of gas properties. NACA Report 1135 does provide charts of the thermally perfect air properties normalized by the calorically perfect air values plotted versus Mach number for select values of total temperature. This approach is limited in application to only diatomic gases (e.g., N_2 , O_2 , and H_2) because of the functional form used to describe the variation of heat capacity with temperature.

Because equation (1) is applicable to only diatomic gases, a different method for computing the one-dimensional compressible flow values of a thermally perfect gas was developed and is described in this paper. This method utilizes a polynomial curve fit of c_p versus temperature to describe the variation of heat capacity for a gas. The data required to generate this curve fit for a given gas can be found in tabulated form in several published sources such as the NBS Tables of Thermal Properties of Gases³ and the JANAF Tables⁴. Actual coefficients for specific types of polynomial curve fits are also available from sources such as NASP TM 1107⁵, NASA SP-3001⁶, and NASA TP 3287⁷. Use of these curve fits based upon tables of standard properties of gases enables the application of this method to any type of gas; monatomic, diatomic, and polyatomic (e.g., H_2O , CO_2 , and CF_4) gases or mixtures thereof, provided a data set of c_p versus temperature exists for the individual gas(es) of interest.

A set of thermally perfect gas equations is derived for the specific heat as a polynomial function of temperature and is presented in the derivation section of this paper. This set of equations was coded into a computer program referred to as the thermally perfect gas (TPG) code, which represents the end product of this research effort. The code is available free from the NASA Langley Software Server (LSS) at URL <http://www.larc.nasa.gov/LSS>. The output tables of the TPG program are structured to

resemble the tables of one-dimensional compressible flow properties that appear in NACA Report 1135. The difference (and advantage) of the output tables from the TPG code is their validity in the thermally perfect temperature regime as well as in the calorically perfect temperature regime. This code serves the function of the tables of NACA Report 1135 for any gas species or mixture of gas species (such as air), and significantly increases the range of valid temperature application due to its thermally perfect analysis.

NOMENCLATURE

Symbols

a	speed of sound
A	cross-sectional area of stream tube or channel
A_j	coefficients of the polynomial curvefit for c_p/R
Beta	$\sqrt{M^2 - 1}$
c_p	specific heat at constant pressure
c_v	specific heat at constant volume
e	internal energy per unit mass
h	enthalpy per unit mass, $e + pv$; Planck's constant
k	Boltzmann constant
M	Mach number, V/a
p	static pressure
q	dynamic pressure, $\rho V^2/2$; heat added per unit mass
R	specific gas constant
T	static temperature
u	velocity component parallel to the free-stream flow direction
v	specific volume, $1/\rho$
V	speed of the flow
W	molecular weight
Y	mass fraction
Δ	increment indicator
γ	ratio of specific heats, c_p/c_v

Θ	molecular vibrational energy constant
ν	characteristic frequency of molecular vibration
ρ	static mass density (RHO)

Subscripts

1	upstream flow reference point; e.g., upstream of shock wave
2	downstream flow reference point; e.g., downstream of shock wave
t	total (stagnation) conditions
*	critical (sonic) conditions
i	i^{th} component gas species of the mixture
j	j^{th} coefficient of the polynomial curve fit for c_p
jmax	the maximum j value
mix	gas mixture
n	total number of gas species that comprise gas mixture
perf	quantity evaluated for gas that is both thermally and calorically perfect.
therm perf	quantity evaluated for a gas that is thermally perfect but calorically imperfect
vib	vibrational contribution

Abbreviations

1-D	one-dimensional
CPG	calorically perfect gas
JANAF	Joint Army-Navy-Air Force
NACA	National Advisory Committee for Aeronautics
NASP	National Aero-Space Plane
NBS	National Bureau of Standards
NTIS	National Technical Information Service
TPG	thermally perfect gas
GUI	graphical user interface
LSS	Langley Software Server

Derivation of Thermally Perfect Equations

Polynomial Curve Fit for c_p

The selection of a suitable curve fit function for c_p is the starting point for the development of thermally perfect compressible flow relations. The form chosen for use in the TPG code was the eight-term, fifth-order polynomial expression given below, where the value of c_p has been nondimensionalized by the specific gas constant.

$$\frac{c_p}{R} = A_1\left(\frac{1}{T^2}\right) + A_2\left(\frac{1}{T}\right) + A_3 + A_4(T) + A_5(T^2) + A_6(T^3) + A_7(T^4) + A_8(T^5) = \sum_{j=1}^8 A_j T^{j-3} \quad (2)$$

A_1 through A_8 are the coefficients of the curve fit for a given temperature range. This is the functional form for c_p used in NASP TM 1107⁵ which provides values of A_1 through A_8 for 15 individual gas species. NASA SP 3001⁶ provides similar c_p/R curve fit coefficient data (A_3 through A_7) for over 200 individual gas species for a five-term, fourth-order polynomial fit equation. NASA TP 3287⁷ also provides similar c_p curve fit coefficient data for 50 reference elements for both a five-term (A_3 - A_7) and a seven-term (A_1 - A_7) fourth-order polynomial fit equation. Equation (2) is valid with this coefficient data also, provided that the coefficients not used are set equal to zero. If the pertinent c_p/R versus temperature data has been fit into some other algebraic expression different from above, that expression could easily be exchanged for equation (2) in the TPG code. The only requirements are that closed-form solutions to both $\int c_p dT$ and $\int (c_p/T) dT$ must be known. The reason for these requirements will become apparent as the compressible flow relations are derived for a thermally perfect gas.

Mixture Properties

The TPG code can be used to compute the thermally perfect gas properties for not only individual gas species but also for mixtures of individual gas species (e.g., air). This capability is achieved in the code by calculating the variation of the heat capacity for the specified gas mixture. The c_p of a mixture of gases is computed from

$$c_{p_{\text{mix}}} = \sum_{i=1}^n Y_i c_{p_i} \quad (3)$$

where Y_i is the mass fraction of the i^{th} gas species. The value of c_{p_i} is determined from equation (2) for each component species. To illustrate how this equation is actually implemented in the code, consider the example of standard air consisting of the four major component species N_2 , O_2 , Ar, and CO_2 .

$$c_{p_{\text{air}}} = Y_{N_2} c_{p_{N_2}} + Y_{O_2} c_{p_{O_2}} + Y_{Ar} c_{p_{Ar}} + Y_{CO_2} c_{p_{CO_2}} \quad (4)$$

Writing this equation in its full form using equation (2) gives

$$\begin{aligned} c_{p_{\text{air}}} = & Y_{N_2} R_{N_2} A_{1_{N_2}} \left(\frac{1}{T^2}\right) + \dots + Y_{N_2} R_{N_2} A_{8_{N_2}} T^5 \\ & + Y_{O_2} R_{O_2} A_{1_{O_2}} \left(\frac{1}{T^2}\right) + \dots + Y_{O_2} R_{O_2} A_{8_{O_2}} T^5 \\ & + Y_{Ar} R_{Ar} A_{1_{Ar}} \left(\frac{1}{T^2}\right) + \dots + Y_{Ar} R_{Ar} A_{8_{Ar}} T^5 \\ & + Y_{CO_2} R_{CO_2} A_{1_{CO_2}} \left(\frac{1}{T^2}\right) + \dots + Y_{CO_2} R_{CO_2} A_{8_{CO_2}} T^5 \end{aligned} \quad (5)$$

By combining like terms in equation (5), a resultant c_p curve for the gas mixture (air) is generated.

$$\begin{aligned} c_{p_{\text{air}}} = & A_{1_{\text{air}}} \left(\frac{1}{T^2}\right) + A_{2_{\text{air}}} \left(\frac{1}{T}\right) + A_{3_{\text{air}}} + A_{4_{\text{air}}} T \\ & + A_{5_{\text{air}}} T^2 + A_{6_{\text{air}}} T^3 + A_{7_{\text{air}}} T^4 + A_{8_{\text{air}}} T^5 \end{aligned} \quad (6a)$$

where

$$\begin{aligned} A_{j_{\text{air}}} = & Y_{N_2} R_{N_2} A_{j_{N_2}} + Y_{O_2} R_{O_2} A_{j_{O_2}} + Y_{Ar} R_{Ar} A_{j_{Ar}} \\ & + Y_{CO_2} R_{CO_2} A_{j_{CO_2}}, \text{ for } j=1,8 \end{aligned} \quad (6b)$$

In generalized terminology equations (6a) and (6b) are expressed as

$$c_{p_{\text{mix}}} = \sum_{j=1}^{j_{\text{max}}} A_{j_{\text{mix}}} T^{j-3} \quad (7a)$$

and

$$A_{j_{\text{mix}}} = \sum_{i=1}^n Y_i R_i A_{j_i}, \text{ for } j=1, j_{\text{max}} \quad (7b)$$

With a known curve fit expression for c_p of the gas mixture, the value of γ for a given temperature can be computed directly from its definition. Mixture properties of gas constant and molecular weight are also computed.

Isentropic Relations

If the flow is assumed to be adiabatic, then the 1-D energy equation written for two separate points

in the flowfield is

$$h_1 + \frac{u_1^2}{2} = h_2 + \frac{u_2^2}{2} \quad (8)$$

where h is the enthalpy and u is the velocity. Using the definition of enthalpy h referenced to 0 K gives

$$\int_0^{T_1} c_p dT + \frac{u_1^2}{2} = \int_0^{T_2} c_p dT + \frac{u_2^2}{2} \quad (9)$$

If point 2 is selected to represent the stagnation condition, then $u_2=0$ and $T_2=T_t$. Then equation (9) reduces to

$$\frac{u_1^2}{2} = \int_0^{T_t} c_p dT - \int_0^{T_1} c_p dT = \int_{T_1}^{T_t} c_p dT \quad (10)$$

where for the selected fifth-order curve fit for c_p (equations 7a and 7b with $j_{\max} = 8$)

$$\begin{aligned} \int_{T_1}^{T_t} c_p dT = & -A_1 \left(\frac{1}{T_t} - \frac{1}{T_1} \right) + A_2 \ln \frac{T_t}{T_1} + A_3 (T_t - T_1) \\ & + \frac{A_4}{2} (T_t^2 - T_1^2) + \frac{A_5}{3} (T_t^3 - T_1^3) + \frac{A_6}{4} (T_t^4 - T_1^4) \\ & + \frac{A_7}{5} (T_t^5 - T_1^5) + \frac{A_8}{6} (T_t^6 - T_1^6) \end{aligned} \quad (11)$$

For a specified total temperature, the value of equation (11) can be computed for a range of static temperatures. Each value of static temperature, T_1 (T_1 less than T_t), represents a unique point in the expansion of the gas from its stagnation conditions. With knowledge of γ , and the speed of sound ($a^2 = \gamma RT$), along with u_1 from equation (10), the Mach number is obtained.

An expression for the static to total pressure ratio p_1/p_t is obtained through the use of the first law of thermodynamics, the definitions of enthalpy and entropy, the equation of state, and the assumption of isentropic flow⁸.

$$\frac{p_1}{p_t} = \frac{1}{\exp \left(\frac{1}{R} \int_{T_1}^{T_t} \frac{c_p}{T} dT \right)} \quad (12)$$

For the selected fifth-order curve fit for c_p , the closed form solution to the integral in equation (12) is

$$\begin{aligned} \int_{T_1}^{T_t} \frac{c_p}{T} dT = & -\frac{A_1}{2} \left(\frac{1}{T_t^2} - \frac{1}{T_1^2} \right) - A_2 \left(\frac{1}{T_t} - \frac{1}{T_1} \right) + A_3 \ln \frac{T_t}{T_1} \\ & + A_4 (T_t - T_1) + \frac{A_5}{2} (T_t^2 - T_1^2) + \frac{A_6}{3} (T_t^3 - T_1^3) \\ & + \frac{A_7}{4} (T_t^4 - T_1^4) + \frac{A_8}{5} (T_t^5 - T_1^5) \end{aligned} \quad (13)$$

Equations (12) and (13) are used in the TPG code to compute the value of p_1/p_t for each value of T_1 . Detailed derivations of thermally perfect relations for the remaining isentropic properties of q_1/p_t (dynamic to total pressure ratio), ρ_1/ρ_t (static to total density ratio), and A_1/A_* (local to sonic area ratio) are given in NASA TP 3447⁸.

Normal Shock Relations

The continuity and momentum equations for 1-D flow across a normal shock wave in a shock-fixed coordinate system are given in equations (14) and (15), respectively.

$$\rho_1 u_1 = \rho_2 u_2 \quad (14)$$

$$p_1 + \rho_1 u_1^2 = p_2 + \rho_2 u_2^2 \quad (15)$$

Dividing the momentum equation by the continuity equation gives

$$\frac{p_1}{\rho_1 u_1} + u_1 = \frac{p_2}{\rho_2 u_2} + u_2 \quad (16)$$

The relation for the speed of sound can be written using the equation of state as

$$a^2 = \frac{\gamma p}{\rho} \quad (17)$$

Solving equation (17) for p and substituting into equation (16) yields

$$\frac{a_1^2}{\gamma_1 u_1} + u_1 = \frac{a_2^2}{\gamma_2 u_2} + u_2 \quad (18)$$

Equation (18) provides the needed relationship across the shock. For a given value of T_1 the left-hand side of equation (18) is known from previous computations. The right-hand side of equation (18) appears to have three unknowns γ_2 , u_2 , and a_2 , but in reality these three variables are all functions of only T_2 . (Actually u_2 depends on both T_2 and T_{t2} , but because a shock wave is considered adiabatic, $h_{t2}=h_{t1}$. This translates to $T_{t2}=T_{t1}$ for a thermally perfect gas because c_p is a function of temperature only.) Therefore, the right-hand side of equation (18) can be expressed as one elementary, nonlinear function of T_2 . An iterative technique has been implemented in the TPG code to solve equation (18) for T_2 . With the

known value of T_2 , the values of γ_2 , u_2 , a_2 , and M_2 are computed in the same manner as γ , u_1 , a_1 , and M_1 were determined for T_1 . The desired shock relations, T_2/T_1 and u_2/u_1 , can then be computed. The expressions for the static pressure and density ratios across the shock, obtained using equations (14), (15), and (17), are presented in equations (19) and (20), respectively⁸.

$$\frac{p_2}{p_1} = 1 + \gamma_1 M_1^2 \left(1 - \frac{u_2}{u_1} \right) \quad (19)$$

$$\frac{\rho_2}{\rho_1} = \frac{u_1}{u_2} \quad (20)$$

Combinations of previously determined static and total pressure ratios yield expressions for the total pressure ratio across the shock and the pitot-static pressure ratio.

$$\frac{p_{t_2}}{p_{t_1}} = \left(\frac{p_{t_2}}{p_2} \right) \left(\frac{p_2}{p_1} \right) \left(\frac{p_1}{p_{t_1}} \right) \quad (21)$$

$$\frac{p_1}{p_{t_2}} = \left(\frac{p_{t_1}}{p_1} \right) \left(\frac{p_1}{p_{t_2}} \right) \quad (22)$$

TPG Code Description

An interactive FORTRAN computer code, herein referred to as the TPG code, has been written based on the equations described previously. The code delivers complete tables of results within seconds when run on a computer workstation or personal computer. The purpose and primary output of the code is the creation of tables of compressible flow properties for a thermally perfect gas or mixture of gases, styled after the tables found in NACA Report 1135. Both the isentropic and normal shock properties may be computed, with tabular entries based upon constant decrements of static temperature or constant increments of Mach number. Such entries in terms of static temperature decrements reveal a fundamental difference between the data of the TPG code and NACA Report 1135. This fundamental difference is highlighted when the TPG code output tables are compared with the calorically perfect gas table of NACA Report 1135, a single table of compressible flow properties for air as a function of Mach number. The properties of thermally perfect

gases vary with both total temperature T_t and local static temperature T rather than with only the ratio of T/T_t . Thus, the utility of the code is its capability to generate tables of compressible flow properties for any total conditions over any range of static temperatures ($T < T_t$, of course) or Mach numbers. In this section the major segments of the TPG code, Version 2.4, along with the various types of output are described. A complete description of the TPG FORTRAN code (Version 2.2) is given in NASA TP 3447⁸.

A graphical-user-interface (GUI) version of the TPG code has also been developed for a Sun Microsystems workstation, requiring the same inputs and generating the same outputs. The mathematical algorithms are identical to the FORTRAN version. This GUI version is described briefly at the end of this section.

The FORTRAN code consists of a *Main* program, three “include” files, several subroutines, and a *Block Data* initialization routine. The subroutines are grouped according to purpose within several files, and are called as needed from various locations within the *Main* program, as well as other subroutines. Table 1 summarizes the files and subroutines which comprise the TPG code. A Unix Makefile has been developed for compilation of the code and creation of an executable file. Defaults are provided for all inputs and a complete execution requires, at a minimum, answering each interactive prompt with a comma, followed by a “carriage return”. Such a minimal execution generates a single output file containing a table of the basic isentropic properties for the standard composition of air. More extensive tables, tables for other gas mixtures, or files for post-processing require specific inputs.

The FORTRAN source code, the GUI executable for Sun Microsystems workstations, and several thermodynamic database files are available in a Unix tar file from the LSS.

The Main Program

The first part of the *Main* program contains the interactive inquiries and responses which specify the gas components, the desired total temperature, and the desired outputs and output formats. The first response required is an identifier character string (an ID), or symbol name, for inclusion within output files. A default ID may be specified, in which case the next three

Table 1. TPG code: Version 2.4 files and subroutines

<u>Files:</u>	<u>Contents:</u>
TPG.f	<i>Main Program</i>
Version.h	Include Code Version Identifier
params.h	Include Parameters
dimens.h	Include Common Blocks
trangej.f	Subroutine <i>trangej</i>
cpsubs.f	Subroutines <i>cpeval</i> , <i>cpNtgra</i> , and <i>cptNtgr</i>
ntgrat.f	Subroutines <i>intCp</i> and <i>intCpT</i>
titer.f	Subroutines <i>t1iter</i> and <i>t2iter</i>
Cratio.f	Subroutine <i>Cratio</i>
initd.f	Subroutine <i>initd</i> and <i>Block Data</i>

questions are omitted, and defaults are assumed. A particular database file may be specified next, describing the necessary thermochemical data for the gases of interest. The contents of such a database file are described in later paragraphs. The code contains a default database necessary to define a four species mixture of air. The gas mixture definition is completed by specification of the number of individual species and the corresponding mass fractions, in the order of the species within the database. Defaults correspond to the standard composition of air. Error checking is incorporated within the code to ensure that the sum of the mass fractions equals unity, and that the database contains sufficient information for the requested case.

The next inputs define the composition and format of the table(s). The total temperature specifies the upper temperature limit output (for which the Mach number is zero). Following that is an input that specifies whether the tables are to be in terms of static temperature or Mach number increments. The default entries in the table(s) are given for incremental Mach numbers over a particular range. Isentropic properties are always included in the table, and normal shock properties may be included as an option. The normal shock properties may be output in the same table as the isentropic properties in a wide

format, or may be output separately, in a second table cross-referenced to the isentropic properties by the Mach number and static temperature. The table of normal shock properties begins with sonic conditions and includes all supersonic entries. The tables are written to an output file by default since they can be rather extensive; however, they may be written to standard output. The TPG code also provides options for additional output files for plotting/postprocessing purposes.

A program loop over the temperature or Mach range between the desired limits computes the basic isentropic properties. A second loop over all supersonic Mach numbers calculates the normal shock properties. After this loop is completed, the data are written to the tables and to a basic postprocessor file. Finally, normalization of the thermally perfect data with that of a calorically perfect gas is performed, and the normalized results may be output to a second postprocessor file. Warning summaries of the number of times the valid polynomial curve fit temperature ranges have been exceeded during the calculations comprise the final output. These warnings, if any, are related to the database information.

Include (or Header) Files

The **Version.h** file contains a character variable specifying the current version number of the computer code which is output at the beginning of each interactive execution, and in the table header. Two files, **params.h** and **dimens.h**, contain information which determine the size of the computer memory required to execute the TPG code, and, thus, the size of the case which may be specified. The dimensions of the primary arrays within the code are included in a FORTRAN parameter statement in **params.h** and have the following values as released in Version 2.4:

<i>mtrm</i> (=8) :	number of polynomial terms which define the relationship for c_p/R ,
<i>mssc</i> (=25) :	maximum number of gas species allowed,
<i>mcvf</i> (=3) :	maximum number of temperature ranges per species allowed and corresponding sets of polynomial coefficients,

mtncr (=10000) : maximum number of
computed static
temperatures.

All values assigned to the preceding parameters, except *mtrm*, may be changed to suit particular user requirements. A change in *mtrm* may require coding changes in the subroutines which perform specific calculations using the $c_p(T)/R$ relationships. The **dimens.h** file specifies common blocks containing all of the major arrays that are dependent on the parameters described above.

Temperature Rangefinder Subroutine

A single function accurately describing the relationship between heat capacity and static temperature over a wide temperature range for typical gases is extremely difficult to define. Multiple polynomial functions over limited temperature ranges are defined much more easily, even while maintaining continuity and smoothness at the interfaces between individual ranges. References 5-7 provide such polynomial curve fits of the specific heat, specific enthalpy per temperature, and specific entropy for a number of gases over multiple temperature ranges. The *trangej* subroutine determines the appropriate temperature range in which the expression for specific heat is to be evaluated. Given a particular temperature, the routine selects the correct temperature range from the set of valid ranges for the gas mixture. In the case of a temperature beyond the limits of any range, the closest range is specified for extrapolation, and a warning message is output for that particular temperature. A single extrapolation warning message is written at the end of the tabular file stating the temperature below, or above, which extrapolations were performed. This warning message appears when any of the component species of a gas mixture require extrapolation.

Polynomial Summation and Integration Subroutines

The equations defined in the derivation section require evaluation of c_p , the integral of c_p , and the integral of c_p/T . These evaluations are performed numerically in three subroutines: *cpeval*, *cpNtgra*, and *cptNtgr*. These routines assume a polynomial expression of the form given in equation (7a). The smallest power of T is -2. The largest power of T must be at least +2,

thus requiring the parameter *mtrm* to be at least 5. Any *mtrm* of 5 or greater may be set in **params.h** with no changes required in the FORTRAN code. However, for *mtrm* < 5, or for a different expression defining c_p/R , these three subroutines must be modified. Increasing *mtrm* beyond the code's release value of 8 would include higher order powers of T (>5) in the polynomials.

Temperature Iteration Subroutines

An expression for Mach number as a function of static temperature results from combining the relationship for the speed of sound within a thermally perfect gas with equation (10) for velocity. Subroutine *t1iter* solves the inverse of this expression, that is, for temperature as a function of Mach number. The nonlinear equation is solved by means of a Newton iteration. Subroutine *t2iter* implements a second Newton iteration to solve equation (18) for the static temperature T_2 behind a normal shock.

Calorically Perfect Comparison

Subroutine *Cratio* may be called after all gas properties have been computed using the thermally perfect relationships. Given a user-input value of γ , the routine uses the appropriate equations from NACA Report 1135 to compute corresponding gas properties for a calorically perfect gas. Each property computed by the thermally perfect equations is normalized by the calorically perfect value to allow analysis of the magnitude of the thermal dependency.

Database File Format

The thermochemical data required by the TPG code for a given mixture of gases is defined in a database file to be read at execution time. A database for the standard composition of air is contained within the code and may be accessed as the default. However, for mixtures of other gases, or more complete models of air, a separate database file may be provided. The format is simple, grouped by species with a two-line header, and additional databases are easily constructed. A sample two-species database is shown in Table 2, with line numbers added (*in italics*) for reference.

Line 1 is a descriptor of the data to follow on line 2, and, as such, is merely a comment line. Line 2 gives the number of species for which the file includes thermochemical data, and the number of temperature ranges over which

Table 2. Sample thermochemical database file

(1)	# of species	#of Temperature ranges : NASP TM 1107 + Mods.
(2)	2	2
(3)	Name: Molecular Wt.	
(4)	N2	28.0160
(5)	tmin	tmax
(6)	20.	1000.
(7)	Cp/R Coefficients: c1(-2) --> c1(5)	
(8)	-1.33984200E+01	1.34280300E+00 3.45742000E+00 5.74727600E-04
(9)	-3.21711900E-06	7.50775400E-09 -5.90150500E-12 1.50979900E-15
(10)	tmin	tmax
(11)	1000.	6000.
(12)	Cp/R Coefficients: c2(-2) --> c2(5)	
(13)	5.87702841E+05	-2.23921563E+03 6.06686971E+00 -6.13957913E-04
(14)	1.49178026E-07	-1.92307130E-11 1.06193594E-15 0.00000000E+00
(15)	Name: Molecular Wt.	
(16)	O2	32.0000
(17)	tmin	tmax
(18)	30.	1000.
(19)	Cp/R Coefficients: c1(-2) --> c1(5)	
(20)	3.88517500E+01	-2.70630800E+00 3.56119600E+00 -3.32782400E-04
(21)	-1.18148000E-06	1.10853500E-08 -1.49299400E-11 5.99553800E-15
(22)	tmin	tmax
(23)	1000.	6000.
(24)	Cp/R Coefficients: c2(-2) --> c2(5)	
(25)	-1.05642070E+06	2.41123849E+03 1.73474238E+00 1.31512292E-03
(26)	-2.29995151E-07	2.13144378E-01 -7.87498771E-16 0.00000000E+00

separate polynomials define c_p/R as a function of T . These integer values are read in free format. Version 2.4 of the code requires that, for each species within a particular file, each of the polynomials must have the same limiting temperatures for each range, except the absolute minimum and maximum temperatures of the overall definition. That is, if the polynomials for one gas are valid from 200 K to 1000 K, and from 1000 K to 5000 K, then each gas within that database file must also be defined by one polynomial up to 1000 K, and a second one above 1000 K. The absolute extrema of 200 K and 5000 K are not required to be identical since the code simply extrapolates the polynomials beyond these limits. Extrapolation warnings are given based upon the worst case, that is, based upon the extrema limits of the most conservatively defined gas.

Lines 3-14 are repeated for each gaseous species in the file. Error handling has been incorporated within the code to recognize *End-of-File* on most computers, without terminating execution, for the case in which the actual

number of species defined is less than expected.

The thermochemical data for the first gas begins with line 3 which again is a descriptor for the next line of data. Line 4 contains the name and molecular weight of the gas. Each temperature range polynomial definition follows, beginning with the lowest. Line 6 gives the minimum and maximum temperatures for the first polynomial. Following another descriptor line, the coefficients A_1 to A_8 (or A_{mtrm} if *mtrm* is not equal to 8) for the polynomial are given in free format on lines 8-9. The minimum and maximum temperatures for the second polynomial are given on line 11, and a second set of coefficients follows on lines 13-14. The pattern is repeated for all the temperature ranges as specified in the database header. The data for a second gas follows directly (lines 15-26), in the same format as the first, and so on until all gases have been defined.

The TPG code uses the gas definitions in the order specified within the database file, and mass fraction inputs must be in that same order. However, mass fractions of zero are acceptable

inputs, if it is desired to omit one or more of the leading species within a given file. Also, the polynomial coefficients for a particular gas do not all have to be nonzero. In particular, a calorically perfect gas may be defined by a database in which all of the coefficients are zero, except A_3 which equals the caloric constant for c_p/R .

Database files provided with the code as currently released on the NASA Langley Software Server contain curve fit definitions for the following gas species: N_2 , O_2 , Ar, CO_2 , H_2O , NO, H_2 , OH, H, O, CF_4 , SF_6 , CH_4 , and calorically perfect air. Multiple curve fit definitions, having different temperature ranges and varying polynomial orders, are provided for some of these gas species.

Graphical User Interface version

A second version of the TPG code utilizes a Motif-based X-window graphical user interface for specification of the user inputs, thus replacing the interactive question-and-answer portion of the program with a point&click window. Currently, this version of TPG only runs on a Sun Microsystems workstation under the Unix operating system. Built using standard Motif widgets and the matrix widgets from the Bellcore Application Environment library, the primary window has pull-down "File" and "Help" menus, and five subwindow regions (see Fig. 1). Along the top are text regions to accept the case ID and a database file name; the latter may be specified by typing or through a file browser. A handy "Compute" button activates the algorithmic loops when proper inputs are provided.

The majority of the GUI window consists of four subregions which allow specification of: 1) the gas species mixture, 2) the total temperature and the tabular limits in terms of temperature or Mach number, 3) optional normal shock output, table formats, and postprocessor files, and 4) the destinations of the tabular outputs. As in the FORTRAN version, defaults are provided for all inputs; however, unlike the interactive FORTRAN version, no user-action is required to accept these defaults. In addition, the GUI has several capabilities not found in the FORTRAN code. Specific output file names may be specified in place of the defaults, and the species mixtures may be specified in terms of either mass or mole fraction. The output may be previewed in a separate on-screen window prior to writing the

tables to a file. Finally, through the use of the file browser a user can be sure that the desired database file does exist, and the associated species are displayed along with their mass or mole fraction. User-error is minimized since error checking is performed prior to calling the isentropic and normal shock algorithmic loops.

The GUI is written in the C programming language and calls a FORTRAN subroutine when the "Compute" button is clicked, if all the inputs meet error-checking criteria. The main FORTRAN subroutine basically consists of the *Main* program from the FORTRAN version of TPG, with the interactive input removed. When "Compute" is selected, the GUI writes a temporary file with all data needed for the FORTRAN code. The remainder of the FORTRAN code is identical to that of the interactive version, except that control returns to the GUI after the "Compute" operation is complete; thus repeated calculations are allowed within a single session.

Comparison to NACA Report 1135

Calorically Perfect Temperature Regime

The TPG code was compared to NACA Report 1135 to verify the code's accuracy in the calorically perfect temperature regime using air as the test gas. In this temperature regime the specific heat of air is nearly constant and the TPG code results should be nearly identical to the tables of NACA Report 1135. For this test case the default data file for standard four-species air was used along with the default values for the mass fraction composition of air. A stagnation temperature of 400 K was selected. This case was run using the Mach number increment option (as opposed to temperature increment) with a Mach number increment of 0.1, a minimum Mach number of 0.0 (the default value), and a maximum Mach number of 3.0. A portion of the **TPG.out** file for this test case is given in Table 3. A comparison of this output with Tables I and II from NACA Report 1135 for any matching Mach number shows the desired agreement and validates the TPG code in this calorically perfect temperature regime. The small differences that are observed between the corresponding values of Table 3 and the NACA Report 1135 tables are in either the third or fourth digit. To better examine these small differences the TPG code was used to generate

the ratio of the gas properties calculated with the thermally perfect relations (Table 3) to those calculated from the calorically perfect relations (NACA Report 1135 tables). These results have been plotted versus Mach number in figures 2 and 3. From these figures the maximum difference between the values listed in Table 3 and the NACA Report 1135 tables appears to be roughly 0.5 percent. Note that these small differences actually represent the small amount of error associated with the tabulated values of NACA Report 1135 resulting from the calorically perfect gas assumption. Close inspection of Table 3 reveals that a slight variation with temperature actually exists in the specific heat ratio which leads to the noted differences when compared with the calorically perfect gas properties.

Thermally Perfect Temperature Regime

The first step in verifying the TPG code in the thermally perfect temperature regime was to compare the γ variation for air computed by the TPG code with both the γ variation calculated from NACA Report 1135 (equation (180)¹) and the theoretical thermally perfect γ variation from the JANAF Thermochemical Tables⁴ (obtained from the theoretical c_p data for N_2 , O_2 , Ar, and CO_2). The variation of γ as a function of temperature is presented in figure 4. Below 300 K, the NACA Report 1135 predicted γ values have attained their asymptotic value of 1.400 while the γ values predicted by the TPG code have reached a slightly greater asymptotic value of 1.401 which is in agreement with the theoretical data⁴. Above 300 K, both the TPG code and the NACA Report 1135 exponential expression for γ produce a nearly identical γ variation that is in excellent agreement with the theoretical γ values up to approximately 1600 K, at which point the γ curve of NACA Report 1135 begins a gradual divergence away from the TPG code γ curve and the theoretical results. This divergence is due to the inability of the NACA Report 1135 exponential expression for γ to accurately model the true thermally perfect behavior of the gas at the higher temperatures. Equation (180)¹ only accounts for the harmonic contribution to the vibrational energy mode. At these higher temperatures (>1600 K) other contributions to the vibrational energy mode, such as anharmonicity and vibrational-rotational interactions, must also be included. The TPG code avoids this limitation by

utilization of multiple-range polynomial curve fits of theoretical data³⁻⁷ to model the variation of heat capacity, which for this particular application of the code consisted of two fifth-order, eight-term polynomial curve fits. Note that, although figure 4 gives thermally perfect results for air up to 3000 K, in reality dissociation of O_2 begins at approximately 1500 K, thus making air thermally imperfect due to a changing composition which is a function of both pressure and temperature.

The remaining gas properties computed by the TPG code in the thermally perfect temperature regime were verified for test cases at total temperatures of 556 K (1000° R), 1111 K (2000° R), 1667 K (3000° R), and 2778 K (5000° R), all with air (using the standard four-species composition) as the test gas. These four specific test cases were selected so that a comparison could be made with the caloric imperfection charts of NACA Report 1135 which give the compressible flow gas properties for air computed from the thermally perfect relations based upon equation (1) of this paper. Each of the twelve charts from NACA Report 1135 gives the variation of one gas property, normalized by its calorically perfect value, versus Mach number for the above mentioned four total temperatures. The TPG code results for these four test cases were also normalized by their calorically perfect values and then plotted together with the results from the caloric imperfection charts of NACA Report 1135. (The results of NACA Report 1135 have been regenerated here for plotting purposes from equations (180-194)¹.) Only two of these twelve charts are presented here due to length considerations, but these two charts (Figures 5 and 6) are typical of the agreement present for all twelve flow properties. Examination of figures 5 and 6 (which correspond to charts 12 and 17 of NACA Report 1135) show that good overall agreement exists (maximum difference less than one percent) for the compressible flow properties computed from the two different thermally perfect methods. The small differences that are observed in these figures can be attributed in most cases to one of the two sources of γ inaccuracies noted previously. One difference noted in figures 5 and 6 is between the curves of the TPG code and NACA Report 1135 for the test case at a total temperature of 2778 K (5000° R). This difference is discernible from the start of the expansion and results from the difference in the

predicted γ values between the two methods for temperatures above approximately 1600 K. (See figure 4.) The other discernible difference between the curves of the TPG code and NACA Report 1135 occurs at all four total temperatures. At some given value of Mach number the curves of the TPG code diverge slightly from the asymptotic plateau value of NACA Report 1135. Examination of the tabular data for these test cases (not included in this report) revealed that the divergence onset Mach numbers for the above stated four test cases all correspond to a static temperature value of approximately 200 K. The divergence between the TPG code and NACA Report 1135 curves which becomes discernible in the plotted data around 200 K is actually a consequence of the difference in the predicted γ values as shown in the low-temperature range of figure 4. This comparison verifies the TPG code accuracy and the derived thermally perfect gas relations based upon polynomial expressions for c_p . Although these test cases were all for air, a primarily diatomic gas, the validation of the TPG code also stands for polyatomic gases. The utilization of a polynomial curve fit for c_p makes the TPG code independent of the molecular structure of the gas⁸.

Comparative Assessment

The TPG code represents a significant advancement over NACA Report 1135 in the compressible flow analysis of both calorically perfect and thermally perfect gases. It is applicable to any type of gas or mixture of gases, unlike NACA Report 1135 whose thermally perfect analysis is only applicable to diatomic gases. The code also has the capability to compute the γ of any arbitrary gas mixture, a feature not provided by NACA Report 1135. Table 4 presents a sample case of hydrogen and air combustion products to illustrate the potential applicability of the TPG code. In both the calorically and thermally perfect temperature regimes the TPG code has been shown to produce more accurate results than NACA Report 1135. The TPG code user need not be concerned with exceeding the temperature limits of the calorically perfect gas assumption for a given gas and therefore is not confronted with a decision of which analysis method to use as is the user of NACA Report 1135. (The user must still be aware of the limits of the thermally perfect gas assumption for each gas within the

mixture.) User-specified tabulated results are available from the TPG code as opposed to caloric imperfection charts found in NACA Report 1135 which require graphical interpolation among four discrete total temperature values. These charts also are only available for air. For other diatomic gases the user of NACA Report 1135 must resort to the set of lengthy exponential equations some of which are implicit. Lastly, the TPG code is easily accessible with the code being available free via the LSS on Internet. These assessments are presented in the form of a comparative matrix in table 5.

Conclusions

A set of compressible flow relations for a thermally perfect gas has been derived for a value of c_p expressed as a polynomial function of temperature and developed into a computer program, referred to as the TPG code, which is available free from the NASA Langley Software Server. The code produces tables of compressible flow properties similar to those found in NACA Report 1135¹. Unlike the NACA Report 1135 tables, which are valid only in the calorically perfect temperature regime, the TPG code results are also valid in the thermally perfect temperature regime, giving the TPG code a considerably larger range of temperature application. Accuracy of the TPG code in the calorically perfect temperature regime was verified by comparisons with the NACA Report 1135 tables. In the thermally perfect temperature regime the TPG code was verified by comparisons with results obtained using the NACA Report 1135 method for calculating the thermally perfect compressible flow properties. The TPG code essentially serves the function of the compressible flow tables of NACA Report 1135 while providing thermally perfect results. It is applicable to any type of gas, not restricted to only diatomic gases as is the method of NACA Report 1135. In addition, the TPG code is capable of handling any specified mixture of individual gas species (for which the necessary polynomial curve fit information for c_p is known for each of the component gas species) since the calculation of the pertinent thermochemical mixture properties is performed within the code.

References

1. Ames Research Staff: *Equations, Tables, and Charts for Compressible Flow*. NACA Report 1135, 1953. (Supersedes NACA TN 1428.)
2. Donaldson, Coleman duP.: *Note on the Importance of Imperfect-Gas Effects and Variation of Heat Capacities on the Isentropic Flow of Gases*. NACA RM L8J14, 1948.
3. Hilsenrath, J.; Beckett, C. W.; Benedict, W. S.; Fano, L.; Hoge, H. J.; Masi, J. F.; Nuttall, R. L.; Touloukian, Y. S.; and Woolley, H. W.: "*Tables of Thermal Properties of Gases*," National Bureau of Standards Circular 564, U.S. Dep. Commerce, November 1, 1955.
4. *JANAF Thermochemical Tables*, Second ed., U.S. Standard Reference Data System NSRDS-NBS 37, U.S. Dep. Commerce, June 1971.
5. Rate Constant Committee, NASP High-Speed Propulsion Technology Team: *Hypersonic Combustion Kinetics*. NASP TM 1107, NASP JPO, Wright-Patterson AFB, May 1990.
6. McBride, Bonnie J.; Heimerl Sheldon; Ehlers, Janet G.; and Gordon, Sanford: *Thermodynamic Properties to 6000 K for 210 Substances Involving the First 18 Elements*. NASA SP-3001, 1963.
7. McBride, Bonnie J.; Gordon, Sanford; and Reno, Martin A.: *Thermodynamic Data for Fifty Reference Elements*. NASA TP-3287, January 1993.
8. Witte, David W.; and Tatum, Kenneth E.: *Computer Code for Determination of Thermally Perfect Gas Properties*. NASA TP-3447, September 1994.

Table 3: Test case for the calorically perfect temperature regime

Thermally Perfect Gas Properties Code TPG, Version 2.4.0															
NASA Langley Research Center															
Table of Thermally Perfect Compressible Flow Properties Gaseous Mixture: Air - 4 species (Standard) mixture of N2, O2, Argon and CO2 Database File name: [Default database of Air Mixture]															
Species Names are: N2 , O2 , Argon, CO2 ,															
Species Mass Fractions are: 0.75530 0.23140 0.01290 0.00040															
Species Mole Fractions are: 0.78092 0.20946 0.00935 0.00026															
Mixture Properties: Molecular Weight = 28.9663 Gas Constant = 2.87035E+02 J/(kg*K) Polynomial Coefficients : cp/R = Sum{A(i)*T^(i-2)}															
80.0 < T < 1000.0 degrees K -3.73198210+00 5.41967010-01 3.46935860+00 3.83537980-04 -2.76531300-06 8.18861420-09 -7.73686900-12 2.43487230-15															
1000.0 < T < 6000.0 degrees K 2.37698510+05 -1.24405270+03 5.12666900+00 -2.04006440-04 6.83218010-08 -1.05535420-11 6.64500710-16 0.00000000+00															
Total Temperature = 400.000 K															
M	T(K)	Gamma	P/Pt	RHO/RH0t	T/Tt	Beta	q/Pt	A/A*	V/a*	M2	P2/P1	RH02/RH01	T2/T1	Pt2/Pt1	P1/Pt2
0.000	400.0	1.3949	1.000E+00	1.000E+00	1.0000	1.0000	0.000E+00	infinite	0.00000	** Subsonic: Not Applicable	---	---	---	---	---
0.100	399.2	1.3949	9.931E-01	9.950E-01	0.9980	0.9950	6.926E-03	5.828E+00	0.10923	** Subsonic: Not Applicable	---	---	---	---	---
0.200	396.9	1.3951	9.726E-01	9.803E-01	0.9922	0.9798	2.714E-02	2.966E+00	0.21784	** Subsonic: Not Applicable	---	---	---	---	---
0.300	393.0	1.3953	9.397E-01	9.564E-01	0.9825	0.9539	5.900E-02	2.037E+00	0.32520	** Subsonic: Not Applicable	---	---	---	---	---
0.400	387.7	1.3956	8.959E-01	9.242E-01	0.9693	0.9165	1.000E-01	1.591E+00	0.43073	** Subsonic: Not Applicable	---	---	---	---	---
0.500	381.2	1.3961	8.434E-01	8.851E-01	0.9529	0.8660	1.472E-01	1.341E+00	0.53389	** Subsonic: Not Applicable	---	---	---	---	---
0.600	373.4	1.3965	7.844E-01	8.403E-01	0.9335	0.8000	1.972E-01	1.189E+00	0.63422	** Subsonic: Not Applicable	---	---	---	---	---
0.700	364.6	1.3970	7.213E-01	7.914E-01	0.9115	0.7141	2.469E-01	1.095E+00	0.73129	** Subsonic: Not Applicable	---	---	---	---	---
0.800	355.0	1.3975	6.564E-01	7.397E-01	0.8874	0.6000	2.935E-01	1.038E+00	0.82478	** Subsonic: Not Applicable	---	---	---	---	---
0.900	344.6	1.3980	5.916E-01	6.867E-01	0.8615	0.4359	3.349E-01	1.009E+00	0.91441	** Subsonic: Not Applicable	---	---	---	---	---
1.000	333.7	1.3985	5.285E-01	6.335E-01	0.8343	0.0000	3.695E-01	1.000E+00	1.00000	1.000E+00	1.000E+00	1.000E+00	1.000E+00	1.000E+00	5.285E-01
1.100	322.4	1.3990	4.695E-01	5.811E-01	0.8061	0.4583	3.965E-01	1.008E+00	1.08144	9.118E-01	1.245E+00	1.169E+00	1.065E+00	9.989E-01	4.690E-01
1.200	310.9	1.3994	4.124E-01	5.305E-01	0.7773	0.6633	4.155E-01	1.031E+00	1.15866	8.422E-01	1.514E+00	1.342E+00	1.128E+00	9.928E-01	4.154E-01
1.300	299.3	1.3998	3.608E-01	4.823E-01	0.7482	0.8307	4.268E-01	1.066E+00	1.23169	7.860E-01	1.806E+00	1.517E+00	1.191E+00	9.793E-01	3.685E-01
1.400	287.7	1.4001	3.141E-01	4.368E-01	0.7192	0.9798	4.310E-01	1.115E+00	1.30057	7.398E-01	2.122E+00	1.691E+00	1.254E+00	9.581E-01	3.278E-01
1.500	276.1	1.4004	2.722E-01	3.943E-01	0.6903	1.1180	4.289E-01	1.176E+00	1.36540	7.012E-01	2.461E+00	1.864E+00	1.320E+00	9.296E-01	2.928E-01
1.600	264.8	1.4006	2.351E-01	3.551E-01	0.6620	1.2490	4.214E-01	1.251E+00	1.42631	6.686E-01	2.823E+00	2.034E+00	1.388E+00	8.950E-01	2.627E-01
1.700	253.7	1.4008	2.024E-01	3.191E-01	0.6342	1.3748	4.097E-01	1.338E+00	1.48345	6.408E-01	3.208E+00	2.200E+00	1.458E+00	8.555E-01	2.366E-01
1.800	242.9	1.4010	1.739E-01	2.863E-01	0.6072	1.4967	3.946E-01	1.440E+00	1.53700	6.168E-01	3.617E+00	2.362E+00	1.532E+00	8.124E-01	2.140E-01
1.900	232.4	1.4011	1.491E-01	2.565E-01	0.5811	1.6155	3.770E-01	1.556E+00	1.58713	5.959E-01	4.050E+00	2.519E+00	1.608E+00	7.671E-01	1.943E-01
2.000	222.3	1.4012	1.277E-01	2.297E-01	0.5558	1.7321	3.577E-01	1.688E+00	1.63404	5.777E-01	4.505E+00	2.670E+00	1.688E+00	7.207E-01	1.771E-01
2.100	212.6	1.4012	1.092E-01	2.055E-01	0.5316	1.8466	3.375E-01	1.837E+00	1.67790	5.617E-01	4.984E+00	2.815E+00	1.771E+00	6.740E-01	1.620E-01
2.200	203.3	1.4013	9.341E-02	1.838E-01	0.5083	1.9596	3.168E-01	2.005E+00	1.71892	5.475E-01	5.486E+00	2.954E+00	1.857E+00	6.280E-01	1.487E-01
2.300	194.4	1.4013	7.989E-02	1.644E-01	0.4860	2.0712	2.961E-01	2.193E+00	1.75726	5.349E-01	6.012E+00	3.087E+00	1.947E+00	5.832E-01	1.370E-01
2.400	185.9	1.4013	6.833E-02	1.470E-01	0.4648	2.1817	2.758E-01	2.403E+00	1.79311	5.236E-01	6.561E+00	3.214E+00	2.041E+00	5.401E-01	1.265E-01
2.500	177.8	1.4013	5.848E-02	1.316E-01	0.4445	2.2913	2.561E-01	2.636E+00	1.82664	5.135E-01	7.133E+00	3.336E+00	2.138E+00	4.991E-01	1.172E-01

Table 4: Sample case representing a gas mixture of hydrogen and air combustion products

Thermally Perfect Gas Properties Code TPG, Version 2.4.0															
NASA Langley Research Center															
Table of Thermally Perfect Compressible Flow Properties Gaseous Mixture: Hydrogen and Air Combustion Products Database file name: /home0/witte/TPG_datafiles/CombProd.data															
Species Names are: H2O , N2 , O2 , Ar , NO H2 , OH , H , O ,															
Species Mass Fractions are: 0.23635 0.73510 0.00787 0.01310 0.00492 0.00165 0.00098 0.00002 0.00001															
Species Mole Fractions are: 0.32005 0.64008 0.00600 0.00800 0.00400 0.01997 0.00141 0.00048 0.00002															
Mixture Properties: Molecular Weight = 24.3948 Gas Constant = 3.40825E+02 J/(kg*K) Polynomial Coefficients : cp/R = Sum{A(i)*T^(i-2)}															
200.0 < T < 1000.0 degrees K 3.49819290+02 -1.27551860+01 3.77980920+00 -4.96362980-04 8.45163500-08 3.53186100-09 -3.86303750-12 1.22257090-15															
1000.0 < T < 6000.0 degrees K 7.14601640+05 -2.21639420+03 5.49026360+00 3.72169730-04 -1.31892240-07 1.91444130-11 -9.38831630-16 0.00000000+00															
Total Temperature = 1800.000 K															
M	T(K)	Gamma	P/Pt	RHO/RHOt	T/Tt	Beta	q/Pt	A/A*	V/a*	M2	P2/P1	RHO2/RHO1	T2/T1	Pt2/Pt1	P1/Pt2
0.000	1800.0	1.2615	1.000E+00	1.000E+00	1.0000	1.0000	0.000E+00	infinite	0.00000	** Subsonic: Not Applicable	---	---	---	---	---
0.200	1790.6	1.2618	9.751E-01	9.802E-01	0.9948	0.9798	2.461E-02	3.009E+00	0.21168	** Subsonic: Not Applicable	---	---	---	---	---
0.400	1763.0	1.2628	9.049E-01	9.238E-01	0.9794	0.9165	9.141E-02	1.608E+00	0.42025	** Subsonic: Not Applicable	---	---	---	---	---
0.600	1718.6	1.2644	8.006E-01	8.386E-01	0.9548	0.8000	1.822E-01	1.196E+00	0.62278	** Subsonic: Not Applicable	---	---	---	---	---
0.800	1659.5	1.2667	6.777E-01	7.351E-01	0.9219	0.6000	2.747E-01	1.040E+00	0.81672	** Subsonic: Not Applicable	---	---	---	---	---
1.000	1588.5	1.2697	5.511E-01	6.245E-01	0.8825	0.0000	3.499E-01	1.000E+00	1.00000	1.000E+00	1.000E+00	1.000E+00	1.000E+00	1.000E+00	5.511E-01
1.200	1508.5	1.2734	4.327E-01	5.163E-01	0.8380	0.6633	3.967E-01	1.033E+00	1.17109	8.398E-01	1.496E+00	1.371E+00	1.091E+00	9.924E-01	4.360E-01
1.400	1422.4	1.2779	3.297E-01	4.172E-01	0.7902	0.9798	4.129E-01	1.126E+00	1.32904	7.331E-01	2.086E+00	1.765E+00	1.182E+00	9.551E-01	3.452E-01
1.600	1333.1	1.2830	2.348E-01	3.310E-01	0.7406	1.2490	4.026E-01	1.280E+00	1.47338	6.576E-01	2.769E+00	2.168E+00	1.277E+00	8.859E-01	2.768E-01
1.800	1242.9	1.2888	1.789E-01	2.591E-01	0.6905	1.4967	3.735E-01	1.503E+00	1.60411	6.019E-01	3.550E+00	2.568E+00	1.382E+00	7.943E-01	2.252E-01
2.000	1153.9	1.2952	1.288E-01	2.009E-01	0.6410	1.7321	3.335E-01	1.806E+00	1.72160	5.597E-01	4.428E+00	2.955E+00	1.498E+00	6.922E-01	1.860E-01
2.200	1067.6	1.3021	9.184E-02	1.548E-01	0.5931	1.9596	2.894E-01	2.208E+00	1.82645	5.269E-01	5.406E+00	3.323E+00	1.627E+00	5.898E-01	1.557E-01
2.400	985.4	1.3093	6.521E-02	1.191E-01	0.5474	2.1817	2.459E-01	2.731E+00	1.91948	5.010E-01	6.485E+00	3.667E+00	1.768E+00	4.943E-01	1.319E-01
2.600	907.9	1.3167	4.625E-02	9.170E-02	0.5044	2.4000	2.058E-01	3.402E+00	2.00166	4.803E-01	7.667E+00	3.984E+00	1.924E+00	4.093E-01	1.130E-01
2.800	835.7	1.3242	3.288E-02	7.081E-02	0.4643	2.6153	1.706E-01	4.252E+00	2.07404	4.635E-01	8.952E+00	4.274E+00	2.095E+00	3.364E-01	9.771E-02
3.000	769.1	1.3316	2.348E-02	5.495E-02	0.4273	2.8284	1.407E-01	5.317E+00	2.13763	4.497E-01	1.034E+01	4.536E+00	2.280E+00	7.754E-01	8.524E-02
3.200	707.9	1.3386	1.688E-02	4.291E-02	0.3933	3.0397	1.157E-01	6.634E+00	2.19340	4.384E-01	1.183E+01	4.772E+00	2.480E+00	2.252E-01	7.496E-02
3.400	652.2	1.3450	1.232E-02	3.376E-02	0.3623	3.2496	9.51E-02	8.248E+00	2.24229	4.289E-01	1.343E+01	4.983E+00	2.695E+00	1.843E-01	6.639E-02
3.600	601.7	1.3508	8.950E-03	2.678E-02	0.3343	3.4593	7.894E-02	1.021E+01	2.28519	4.210E-01	1.512E+01	5.172E+00	2.924E+00	1.512E-01	5.921E-02
3.800	555.9	1.3558	6.611E-03	2.141E-02	0.3088	3.6661	6.471E-02	1.256E+01	2.32290	4.143E-01	1.691E+01	5.340E+00	3.167E+00	1.245E-01	5.312E-02
4.000	514.6	1.3600	4.931E-03	1.725E-02	0.2859	3.8730	5.365E-02	1.532E+01	2.35815	4.086E-01	1.880E+01	5.491E+00	3.423E+00	1.029E-01	4.793E-02

Table 5: TPG Code Versus NACA Report 1135 Comparative Matrix

	Thermally Perfect Gas code	NACA Report 1135
Calorically Perfect Gas (CPG):		
a) Applicability	any gas or mixture of gases, γ is computed	only for gas or gas mixture for which constant γ is known
b) Accuracy	<ul style="list-style-type: none"> - accounts for slight caloric imperfections - adjustable Mach number increment & range - no interpolation required 	<ul style="list-style-type: none"> - ignores small caloric imperfections of "realistic" gases - fixed Mach number increment ($\Delta M=0.01$) - interpolation required for improved precision
c) Temperature range	not restricted to CPG limits	restricted to CPG limits
d) Tabulated results	yes, for any gas	yes, only for $\gamma=1.4$
e) Ease-of-use	simple responses to interactive program	table look-up for $\gamma=1.4$, evaluation of CPG equations for $\gamma \neq 1.4$
f) Cost	free via Internet http://www.larc.nasa.gov/LSS	nominal from NTIS
Thermally Perfect Gas (TPG):		
a) Applicability	any gas or mixture of gases: monatomic, diatomic, triatomic, or polyatomic	diatomic gases only
b) Accuracy	user-definable, multi-segment, high order polynomial curve fit	single-parameter, exponential curve fit for diatomic gases only
c) Temperature range	restricted to thermally perfect gas limits	restricted to thermally perfect gas limits
d) Tabulated results	yes, for any gas	no, caloric imperfection charts available for air at 4 discrete total temperatures
e) Ease-of-use	simple responses to interactive program	reading of charts for air, or evaluation of set of implicit, lengthy exponential equations for other diatomic gases
f) Cost	free via Internet: http://www.larc.nasa.gov/LSS	nominal from NTIS

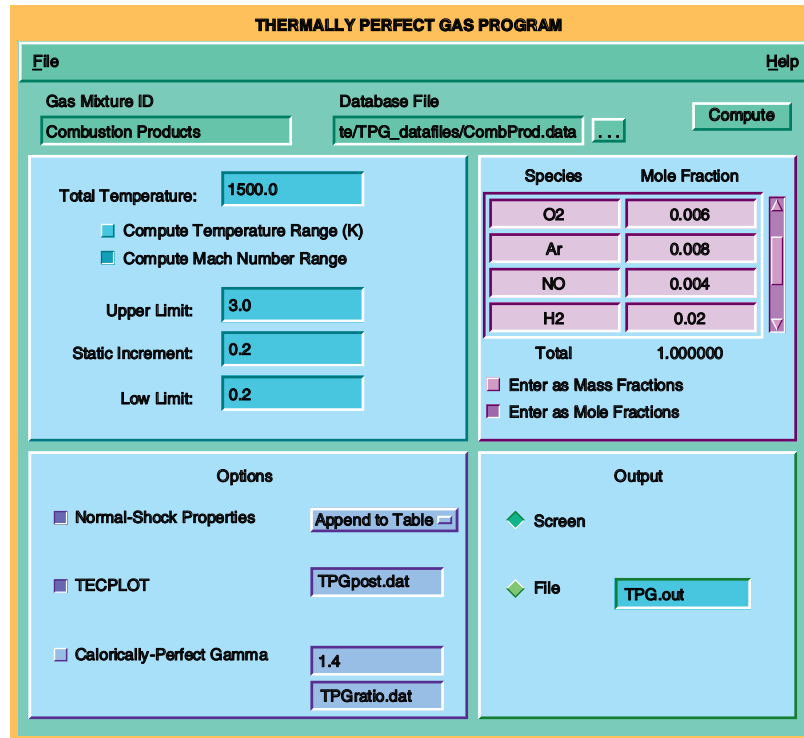


Figure 1. TPG Graphical User Interface

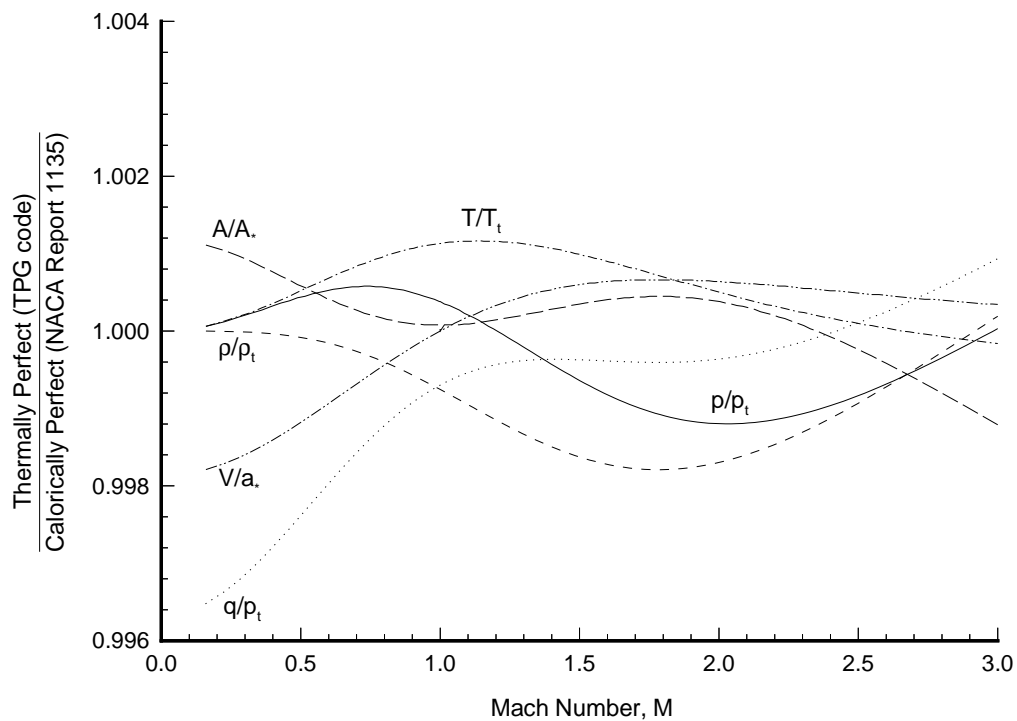


Figure 2. Caloric imperfections of isentropic properties for air ($T_t = 400$ K)

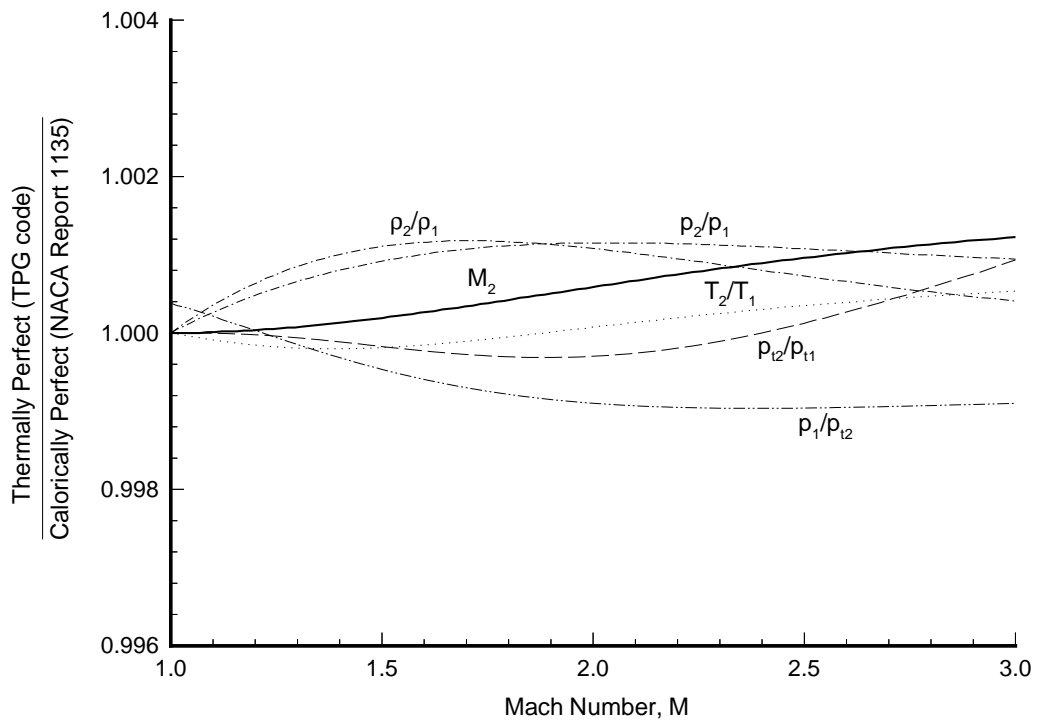


Figure 3. Caloric imperfections of normal shock properties for air ($T_t = 400$ K)

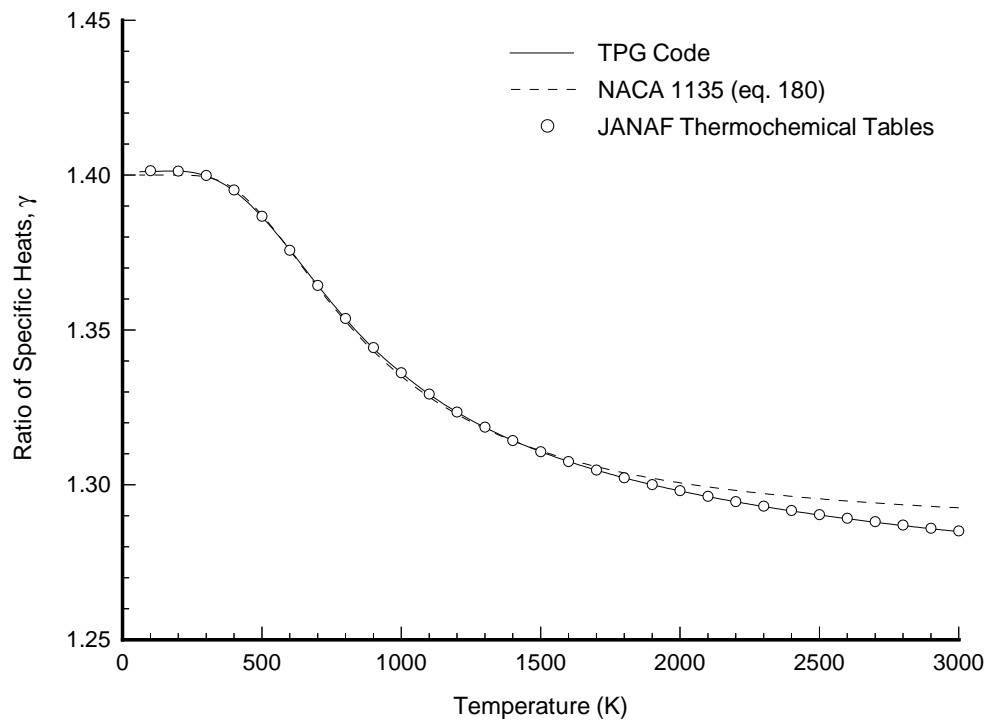


Figure 4. Variation of γ with temperature for thermally perfect air

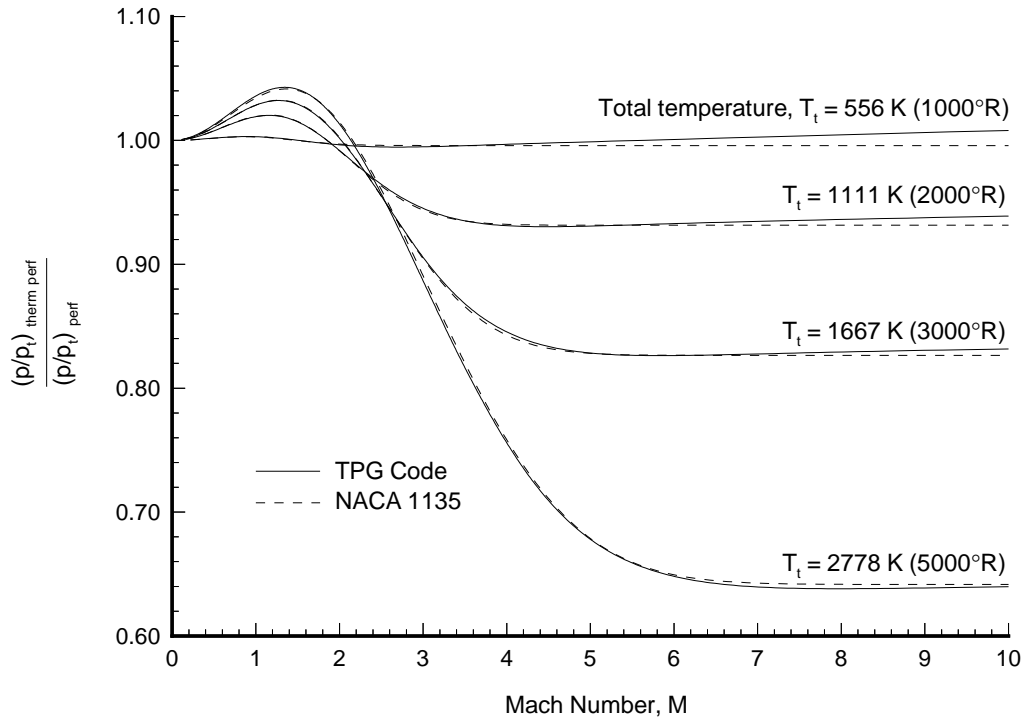


Figure 5. Caloric imperfections of static to total pressure ratio for air

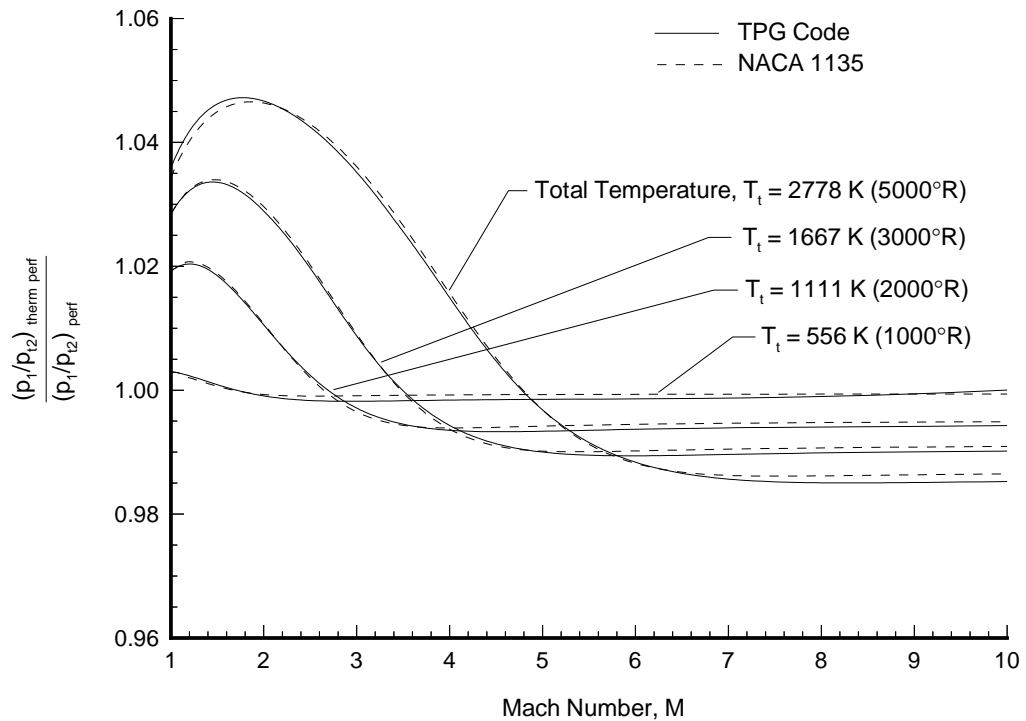


Figure 6. Caloric imperfections of pitot-static pressure ratio for air